Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First principles study of thermal conductance across the MgO/TiN interface DEREK STEWART, SAIKAT MUKHOPADHYAY, Cornell University — MgO and TiN are well lattice-matched crystals and their interface has one of the lowest thermal resistances currently measured. As such, it represents a key test for atomistic models for thermal interfacial resistance. In this work, we examine the phonon contribution to thermal transport across the epitaxial MgO/TiN (001) and (111) interfaces using an atomistic Green's function approach that incorporates interatomic force constants calculated using density functional theory. Since TiN is a metal, this approach will allow us to isolate the direct phonon contribution to thermal conductance across the interface. Calculated phonon dispersions for bulk MgO and TiN show good agreement with experiment. We will discuss how the predicted thermal interface resistance compares with values calculated using standard acoustic mismatch and diffusive mismatch models. We will also examine the impact of TiN nitrogen vacancies on both the bulk phonon dispersion and MgO/TiN thermal conductance.

Derek Stewart
Cornell University

Date submitted: 15 Nov 2013 Electronic form version 1.4